

Generating Synthetic Data Is Complicated: Know Your Data and Know Your Generator

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Abstract. In recent years, more and more synthetic data generators (SDGs) based on various modeling strategies have been implemented as Python libraries or R packages. With this proliferation of ready-made SDGs comes a widely held perception that generating synthetic data is easy. We show that generating synthetic data is a complicated process that requires one to understand both the original dataset as well as the synthetic data generator. We make two contributions to the literature in this topic area. First, we show that it is just as important to pre-process or clean the data as it is to tune the SDG in order to create synthetic data with high levels of utility. Second, we illustrate that it is critical to understand the methodological details of the SDG to be aware of potential pitfalls and to understand for which types of analysis tasks one can expect high levels of analytical validity.

Keywords: Synthetic · Utility · CTGAN · DataSynthesizer · synthpop

1 Introduction

The idea of synthetic microdata⁴ for statistical disclosure limitation was introduced more than 30 years ago [14,8,6] and has become increasingly popular in recent years [5,2]. The general appeal of synthetic data is obvious: synthetic data promises to mimic the statistical properties of the original data while maintaining the confidentiality of individual records. In practice, releasing synthetic data means fitting a model to the original data and then generating new data based on this model.⁵ The new interest in synthetic data was spurred by the develop-

⁴ Throughout the paper, when we refer to data, we are referring to classical microdata (i.e., one observation per individual unit), as opposed to summary tables or images.

⁵ Note that there are different philosophies about the definition of original data and how much pre-processing (e.g., dealing with missing values or outliers) one should do to the original data before data synthesis depending on the synthesis goals (replacement of the original data vs. tool for preparing to work with the original data in a safe environment). In section 3 we describe the data and any pre-processing steps in detail.

2.2 Synthetic data generators (SDGs)

synthpop (Version 1.8.0) [9] is an R package that implements parametric and ML based models (classification and regression trees (CART) and random forests) to generate synthetic data. In our application we use the default settings of the package.⁹ **synthpop** follows a sequential process, where the first variable to be synthesized is generated by drawing new values from the marginal distribution of this variable (either by drawing from a parametric distribution or by sampling from the empirical distribution), and the subsequent variables are synthesized one at a time, always conditioning on those variables that have been synthesized in earlier steps.

DataSynthesizer (Version 0.1.13) [12] is a Python package that implements the PrivBayes algorithm [19]. PrivBayes is designed to address the challenges associated with a differentially private method for releasing synthetic data outputs from high-dimensional real data inputs. To do this, the package implements a Bayesian network model to estimate the joint distribution of the data.

To generate synthetic data from a Bayesian network, the first step is to specify a graphical model (a directed acyclical graph (DAG)) that represents how and in what way the different variables are related to each other. **DataSynthesizer** doesn't require this model structure as input, instead it tries to estimate the optimal structure given the data. As a hyperparameter users can set the maximum number of parents (k) that should be considered for the model. The more parents, the more complex relationships between the variables. After specifying the model and estimating its parameters from the original data, synthetic data are generated by sampling new values based on the probabilities from the model's conditional probability table.

For example, imagine data with four columns (variables) with categorical values: age (young, middle, old), education (less than secondary, secondary, and more than secondary), gender (M and F), and income (low, middle, and high). The number of observations (or rows) are not relevant because the data are transformed into a frequency table with one cell for each unique combination of groups. In this example, there are 54 cells ($3 \times 3 \times 2 \times 3$). If we assume that age, education, and gender are the parents of income, then each value in the conditional probability table represents the conditional probability of each income category given the states of the other three variables. The algorithm calculates the probabilities based on the frequencies from all possible combinations of the variables. To make this model tractable for high dimensional data, the graph structure enforces conditional independence between some of the variables, reducing the number of parameters that need to be estimated. Once the model is defined and parameters are estimated, the Bayesian network generates synthetic data by sampling new values using the estimated probabilities. In our applications, We use default settings except for the number of parents, which we set to

⁹ Default means that CART models are used for synthesis with complexity parameter = 0.001 (smaller values will grow larger trees), and minbucket = 5 (the minimum number of observations in any terminal node).

$k = 2$ (default is "greedy", which means that DataSynthesizers tries to find the optimal value for k).

CTGAN (Version 1.9.0) [17] is a Python package that is part of the Synthetic Data Vault (SDV) package [11]. In their original application, generative adversarial networks (GANs) were designed to create synthetic images [4], but the approach was later adapted to also create synthetic microdata [10]. GANs simultaneously train two neural networks: a generator and a discriminator. The goal of the generator is to create synthetic data that becomes increasingly indistinguishable from original data. The goal of the discriminator is to get better at distinguishing between original and synthetic data. This adversarial process goes back and forth until the discriminator cannot distinguish between the original data and the generated data.

To illustrate how GANs generate synthetic data, imagine we have one variable: income (LN) from Census data with a mean of 10 and a standard deviation of 1. First, the generator network receives random noise vectors as input, typically sampled from a standard normal distribution with mean of 0 and a standard deviation of 1, and sends it to the discriminator to be evaluated. Second, the discriminator evaluates the synthetic data alongside real data to determine the probability that the generated data is real (1) or fake (0). If the discriminator determines that the generated data are fake, it sends feedback to the generator in the form of a loss function. Higher values indicate that it is easier for the discriminator to differentiate between real and fake data. Third, the generator then updates its parameters based on the loss function and the learning rate, which determines the magnitude of this update. The higher the learning rate, the larger the adjustments the generator will make to its parameters in response to the feedback. Fourth, updated data generated from the updated parameters are sent to the discriminator. Ultimately, this back and forth process results in a generator that produces synthetic data that ideally has the same statistical properties as the original data. In our application we mostly rely on default settings except for the number of epochs which we set to 600 (default is 300), but we also vary a number of other hyperparameters, as we explain in detail below.

3 Know your data

SD2011 contain a variety of characteristics found in real data that can present a challenge to synthetic data generators (SDGs). These challenges should be addressed prior to applying a SDG. However, cleaning the data requires knowledge of the data that is not always available to those with knowledge of a given SDG and may not be easy to detect or follow simple rules. We use DataSynthesizer ($k = 2$) to demonstrate the importance of preprocessing the data, but the points raised in this section are applicable to all SDGs.

Missing values. In real data, missing values are sometimes coded as either negative values or large positive values (999999). For example, in the variable `wkabdur` (Months working abroad in 2007-2011) from SD2011, 97.5% of all values are -8. The interpretation is values of -8 represent missing values and only 2.5%

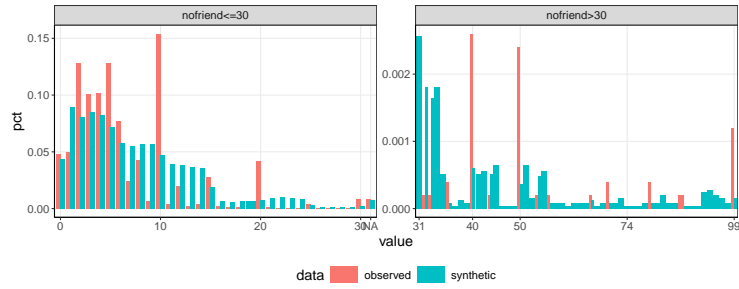


Fig. 4: ‘Spikey’, discontinuous, or semi-continuous distributions can be problematic for SDGs. Here, DataSynthesizer seems to smooth spikes in the variable ‘Number of friends’.

in SD2011 is the variable `nofriend` (number of friends). In the original data, the variable `nofriend` appears to be normally distributed below 10, but then clusters at values of 10, 15, 20 and groups of 10 up to the maximum 99. This phenomenon is sometimes referred to as ‘spikey’, discontinuous, or semi-continuous distributions. As shown in Figure 4 and discussed in more detail below, errors and spikes can pose a problem for statistical utility because most SDGs tend to smooth these spikes unless they are explicitly modeled.

To illustrate the importance of pre-processing the data, we use three versions of the original data to create synthetic data and evaluate the utility of each generated dataset using the pMSE. SD2011(a) is the raw data. SD2011(b) codes all negative values that indicate missing values in numeric variables and all empty values in character variables as missing. SD2011(c) drops the two generated variables (`agegr` and `bmi`) and then recreates them from the synthetic values. Using DataSynthesizer as our SDG and setting the DAG structure to allow a maximum of two parents, the pMSE changes from 0.2 for SD2011(a) to 0.13 for SD2011(b) to 0.07 for SD2011(c). As measured by the pMSE, the improvements in utility are substantial. In fact, when experimenting with the different tuning parameters of the different synthesizers, we found that none of the tuning parameters had such a strong impact on utility as pre-processing the data (results not reported).

4 Know your generator

In this section we discuss the importance of knowing the details of the underlying methodology of the SDG to avoid pitfalls or to at least be aware for which analysis tasks the generated data might offer reasonable analytical validity and for which not. We illustrate this point by providing an example of a methodological aspect for each synthesizer that has important impacts on the synthesis, but that might not be immediately obvious when only considering the general methodology of the SDG.

4.1 synthpop

Categorical variables with large numbers of categories can substantially increase the run-time of CART based synthesizers. To understand why, it is important to understand how CART models are built. CART models operate by finding recursive binary splits to maximize the homogeneity of the values of the dependent variable in the two leaves generated by the split. To find the best possible splits, CART models search over all variables in the dataset. For each variable all possible splits are evaluated and the split that maximizes the homogeneity across all splits and all variables is selected. For continuous and ordered categorical variables the number of splits that needs to be evaluated is $k - 1$, where k is the number of unique values in the variable. This is because each value is considered as a possible splitting criteria with all values less than the value ending up in the left leaf and all other values ending up in the right leaf.

For unordered categorical variables, the number of splits that need to be considered is $2^{L-1} - 1$, where L is the number of categories, i.e., the number of splits grows exponentially with the number of categories. To illustrate, imagine one categorical variable with three values (a, b, and c). There are $2^2 - 1 = 3$ possible options to split this variable: (1 = a; 0 = b,c), (1 = b; 0 = a,c), (1 = c; 0 = a,b). With six categories, we already need to consider 31 splits, which still doesn't pose a problem computationally. However, if there are 20 categories, then 524,288 splits need to be considered. The computational burden can be substantial with even a few categorical variables with a large number of categories.

In the sequential modeling approach that is used with synthpop, each variable that has been synthesized previously is used as a predictor in all subsequent synthesis models. If a variable with many categories is synthesized early during the synthesis process, it will always be used as a predictor for all other synthesis models imposing a high computational burden on the synthesizer. On the other hand, if the variable is the last variable to be synthesized, it will never be used as a predictor, considerably speeding up the synthesis process.

For this reason, it is recommended to synthesize categorical variables with many categories last when using CART models [13]. However, problems arise if there are a sufficient number of variables with a large number of unique values. For example, if a Census data set contained variables for 3-digit ISO country code, 3-digit ISCO codes (occupation), and 3-digit ISIC codes (industry), then it would be difficult to avoid computational problems through ordering.

Other solutions exist, but limitations remain: One option is to aggregate categorical variables with a large number of unique values. However, avoiding the information loss from aggregation is typically one of the reasons to rely on synthetic data to begin with. Alternatively, the categorical variable can be used to stratify the data and to run separate synthesis models within each stratum. Obviously, this will only be an option if the sample sizes in each stratum are still large enough to allow sufficiently rich synthesis models within each stratum.

To illustrate the problem with categorical variables, we examine the duration in time required to create synthetic data using synthpop, i.e. computational efficiency, as shown in table 1. If we load the raw SD2011 into R as a .csv file as

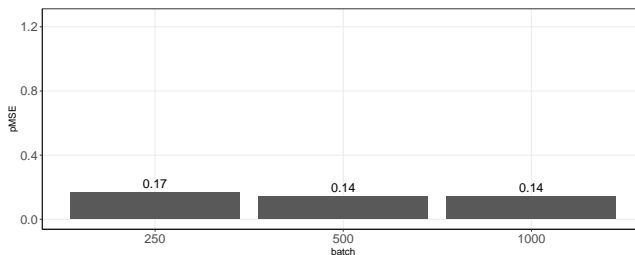


Fig. 6: The relationship between batch size and utility of the synthetic data generated by CTGAN (measured by the pMSE) with the number of training steps held constant (3,000).

computational complexity. Besides, setting the number of bins too high would lead to unstable model estimates, as a very large number of parameters would need to be estimated from the data. Furthermore, if the formal privacy guarantees of DataSynthesizer are turned off as in our application, increasing the number of bins can also lead to increased risks of disclosure. If, on the other hand, the formal guarantees should be maintained when increasing the number of bins, more noise needs to be added to each of the parameters and utility would suffer.

4.3 CTGAN

GANs are designed to work well with continuous variables, but GANs can struggle modeling relationships in micro data because cells in micro data are not informative of neighbors in the same way that pixel cells are in a photograph [2]. CTGAN contains a number of hyperparameters that one can use to tune the model. For this study, we tune the hyperparameters in three main ways. First, we maintain a constant number of iterations (3,000), but allow the batch size to vary, as shown in Figure 6. Second, we maintain a constant batch size (500), but allow the number of iterations to vary, as shown in Figure 7. Third and finally, we vary the dimensionality of the generator/discriminator networks and the embedding dimension, as shown in Figure 8. In our data, tuning these hyperparameters makes little difference (pMSE \approx 0.16). For reference, pMSE from CTGAN is higher than DataSynthesizer (0.07) and synthpop (0.02).

We are aware of other research where tuning hyperparameters does make a difference in the quality of synthetic data output (as yet unpublished). One possible explanation for the fact that hyperparameters do not affect the quality of the synthetic data output is that our data are too low dimensional for the parameters to make a difference. While CTGAN does not produce data with high levels of utility with the data we use here, we do not mean to suggest that GANs are bad SDGs in general. CTGAN is not the only GAN in Synthetic Data Vault and multiple other GANs exist. Based on our own experience, it is possible to create a GAN that provides higher levels of utility. More generally, one must distinguish between the package and the method.

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A Appendix: Utility measures

The **propensity score (pMSE)** is an utility measure that estimates how well one can discriminate between the original and synthetic data based on a classifier [16,15] and is implemented in R from the synthpop package [9]. This is sometimes called a ‘broad’[15] or ‘general’[3] measure of utility or ‘statistical fidelity’ [5]. The main steps are to append or stack the original and the synthetic data, add an indicator (1/0) to distinguish between the two, use a classifier to estimate the propensity of each record in the combined dataset being ‘assigned’ to the original data. The pMSE is the mean squared error of these estimated propensities:

$$pMSE = \frac{1}{N} \sum_{i=1}^N [\hat{p}_i - c]^2 \quad (1)$$

where N is the number of records in the combined dataset, \hat{p}_i is the estimated propensity score for record i , and c is the proportion of data in the merged dataset that is synthetic (in many cases $c = 0.5$). The pMSE can be estimated using all the variables in the dataset, but it can also be computed using subsets of the variables, e.g., all pairwise combinations of variables to evaluate specifically how well the distribution of these variables is preserved. The smaller the pMSE, the higher the analytical validity of the synthetic data.

Computational efficiency is the run time (in seconds) required to create one single synthetic dataset from a given SDG.¹² This is sometimes referred to as ‘efficiency’[5] or ‘output scalability’ [19]. The basic idea is that the algorithms used by SDGs can suffer from the curse of dimensionality.

¹² In terms of computing power, SDGs were run on a 2022 Macbook Air with 16GB of RAM and an M2 Chip with 8-Core CPU, 8-Core GPU, and a 16-Core Neural Engine. All SDGs were run one at a time in order to minimize computational power problems from parallelization.